

Supplementary Information

A Novel and Potent Lewis Acid Catalyst: Br₂-Catalyzed Friedel–Crafts Type Reactions of Naphthols with Aldehydes

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I. General information

Chemicals were all purchased from commercial sources and used without treatment. Thin-layer chromatography (TLC) was carried out using silica gel GF254 plates. Products were purified by column chromatography over silica gel. ^1H NMR and ^{13}C NMR spectra were recorded at 25 °C on a Bruker AscendTM 400 spectrometer in $\text{CDCl}_3/\text{DMSO}$ using TMS as internal standard. High-resolution mass spectra (HRMS) were obtained using a Bruker microTOF II Focus spectrometer (ESI).

Optimization of all molecular geometries, vibrational analyses and Mulliken atomic (MA) charges were calculated at B3LYP¹ and M06-2X² functions with the 6-31+G(d,p)³ and def2-TZVP⁴ basis sets by using Gaussian 09 program. A natural bonding orbital (NBO) analysis for structures was also performed to determine the natural population atomic (NPA) charges by using the NBO 3.1 package implemented in Gaussian 09. All calculated structures were true minima (i.e., no imaginary frequencies). Solvent effect at M06-2X/def2-TZVP level was calculated using the solvent model density (SMD) approach.⁵

II. General procedure

3b as example: To a stirred solution of β -naphthol **1a** (144 mg, 1.0 mmol) and 3-nitrobenzaldehyde **2b** (83 mg, 0.55 mmol) in CH_2Cl_2 (4.0 mL) was added a solution of Br_2 (0.0051 mL) in CH_2Cl_2 (1.0 mL), and the mixture was stirred for 12 h at ambient temperature. After **1a** was consumed, as indicated by TLC, the reaction mixture was quenched with saturated aqueous $\text{Na}_2\text{S}_2\text{O}_3$ (0.5 mL) and water (20.0 mL), and extracted with CH_2Cl_2 four times. The residue obtained after evaporation of the solvent was purified by column chromatography on silica gel (petroleum ether–ethyl acetate = 12:1, v/v) to afford benzylidene biphenol **3b** as an offwhite solid (202 mg, 96% yield).

¹ Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. *J. Phys. Chem.* **1994**, *98*, 11623.

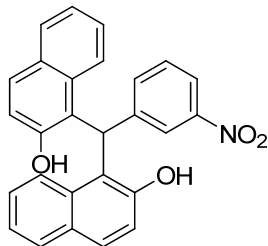
² Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

³ Petersson, G. A.; Bennett, A.; Tensfeldt, T. G.; Al-Laham, M. A.; Shirley, W. A.; Mantzaris, J. *J. Chem. Phys.* **1988**, *89*, 2193.

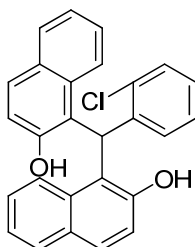
⁴ Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.

⁵ Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2009**, *113*, 6378.

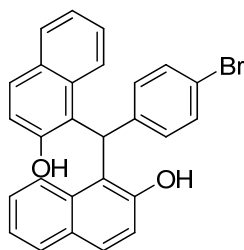
III. Spectral data of new compounds



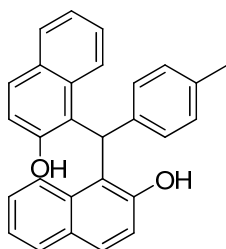
3b, 1,1'-((3-nitrophenyl)methylene)dinaphthalen-2-ol, offwhite solid: mp 174-175 °C (dec.). ^1H NMR (400 MHz, DMSO) δ = 7.10-7.25 (m, 7H), 7.48 (d, J = 4.9 Hz, 2H), 7.70 (d, J = 8.9 Hz, 2H), 7.74 (d, J = 7.7 Hz, 2H), 7.83 (s, 1H), 8.00-8.03 (m, 1H), 8.13 (d, J = 8.5 Hz, 2H), 10.39 (bs, 2H); ^{13}C NMR (100 MHz, DMSO) δ = 154.0, 148.0, 147.7, 135.5, 134.5, 129.4, 128.93, 128.86, 126.5, 123.7, 123.0, 122.5, 120.5, 119.9, 119.5, 41.7; HRMS (ESI-TOF) Calcd for $\text{C}_{27}\text{H}_{20}\text{NO}_4^+$ ($[\text{M}+\text{H}]^+$) 422.1387. Found 422.1393.



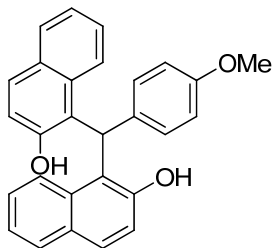
3d, 1,1'-((2-chlorophenyl)methylene)dinaphthalen-2-ol, pinkish solid: mp 200-201 °C (dec.). ^1H NMR (400 MHz, CDCl_3) δ = 5.50 (bs, 1H), 6.61 (bs, 1H), 6.96 (d, J = 8.8 Hz, 1H), 7.04 (d, J = 8.8 Hz, 1H), 7.14-7.18 (m, 2H), 7.20-7.25 (m, 3H), 7.27-7.29 (m, 1H), 7.40 (dd, J = 7.3, 7.5 Hz, 1H), 7.47 (dd, J = 1.0, 7.9 Hz, 1H), 7.53 (dd, J = 7.9, 7.4 Hz, 1H), 7.69-7.75 (m, 4H), 7.85 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.6 Hz, 1H); ^{13}C NMR (100 MHz, DMSO) δ = 153.5, 152.6, 142.7, 134.6, 134.4, 133.9, 131.0, 129.2, 129.1, 128.9, 128.85, 128.76, 127.2, 126.7, 126.5, 126.1, 124.9, 123.4, 122.6, 122.4, 121.2, 119.3, 118.8, 118.7, 110.0, 40.5; HRMS (ESI-TOF) Calcd for $\text{C}_{27}\text{H}_{20}\text{ClO}_2^+$ ($[\text{M}+\text{H}]^+$) 411.1146. Found 411.1150.



3e, 1,1'-((4-bromophenyl)methylene)dinaphthalen-2-ol, yellowish crystal: 192-193 °C (dec.). ^1H NMR (400 MHz, CDCl_3) δ = 6.25 (bs, 2H), 7.01 (s, 1H), 7.02 (d, J = 7.9 Hz, 2H), 7.08 (d, J = 8.3 Hz, 2H), 7.33-7.42 (m, 6H), 7.72 (d, J = 8.8 Hz, 2H), 7.81 (dd, J = 1.5, 7.7 Hz, 2H), 7.88 (d, J = 8.4 Hz, 2H); ^{13}C NMR (100 MHz, DMSO) δ = 153.0, 144.4, 134.5, 130.9, 130.8, 129.14, 129.05, 128.8, 126.3, 124.3, 122.6, 120.3, 119.3, 118.3, 41.4; HRMS (ESI-TOF) Calcd for $\text{C}_{27}\text{H}_{20}\text{BrO}_2^+$ ($[\text{M}+\text{H}]^+$) 455.0641. Found 455.0639.

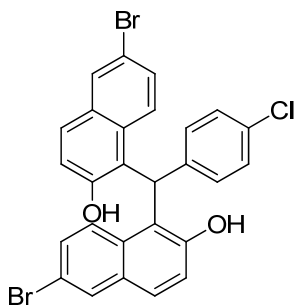


3g, 1,1'-((p-tolyl)methylene)dinaphthalen-2-ol, yellowish solid: 177-178 °C (dec.). ^1H NMR (400 MHz, DMSO) δ = 2.24 (s, 3H), 6.88 (d, J = 8.0 Hz, 2H), 6.98 (d, J = 8.6 Hz, 2H), 6.99 (s, 1H), 7.13 (d, J = 8.8 Hz, 2H), 7.15-7.23 (m, 4H), 7.68 (d, J = 8.8 Hz, 2H), 7.72 (dd, J = 1.8, 7.6 Hz, 2H), 8.10 (d, J = 8.2 Hz, 2H), 9.72 (bs, 2H); ^{13}C NMR (100 MHz, DMSO) δ = 153.1, 141.3, 134.6, 134.3, 129.1, 128.9, 128.85, 128.81, 128.5, 126.3, 124.4, 122.6, 120.9, 119.4, 41.5, 21.0; HRMS (ESI-TOF) Calcd for $\text{C}_{28}\text{H}_{23}\text{O}_2^+$ ($[\text{M}+\text{H}]^+$) 391.1693. Found 391.1696.

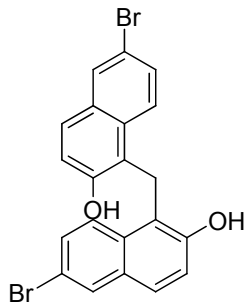


3h, 1,1'-((4-methoxyphenyl)methylene)dinaphthalen-2-ol, offwhite crystal: 195-196 °C (dec.). ^1H NMR (400 MHz, DMSO) δ = 3.68 (s, 3H), 6.75 (d, J = 8.7 Hz, 2H), 6.91 (d, J = 8.5 Hz, 2H), 6.97 (s, 1H), 7.12 (d, J = 8.8 Hz, 2H), 7.16-7.23 (m,

4H), 7.68 (d, $J = 8.9$ Hz, 2H), 7.72 (dd, $J = 1.5, 7.4$ Hz, 2H), 8.09 (d, $J = 8.4$ Hz, 2H), 9.69 (bs, 2H); ^{13}C NMR (100 MHz, DMSO) $\delta = 157.4, 153.1, 136.1, 134.6, 129.5, 129.1, 128.89, 128.85, 126.2, 124.4, 122.6, 121.0, 119.4, 113.6, 55.3, 41.1$; HRMS (ESI-TOF) Calcd for $\text{C}_{28}\text{H}_{23}\text{O}_3^+$ ($[\text{M}+\text{H}]^+$) 407.1642. Found 407.1644.



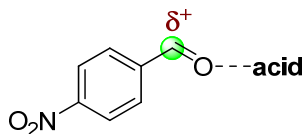
3k, 1,1'-((4-chlorophenyl)methylene)bis(6-bromonaphthalen-2-ol), pinkish solid: 245-246 °C (dec.). ^1H NMR (400 MHz, DMSO) $\delta = 6.96$ (d, $J = 7.0$ Hz, 2H), 6.99 (s, 1H), 7.19 (d, $J = 8.8$ Hz, 2H), 7.24 (d, $J = 8.5$ Hz, 2H), 7.31 (dd, $J = 2.2, 9.3$ Hz, 2H), 7.70 (d, $J = 8.9$ Hz, 2H), 7.97 (d, $J = 9.4$ Hz, 2H), 8.00 (d, $J = 2.1$ Hz, 2H), 10.08 (s, 2H); ^{13}C NMR (100 MHz, DMSO) $\delta = 153.7, 143.2, 133.1, 130.5, 130.4, 130.1, 128.9, 128.6, 128.1, 126.9, 120.6, 120.4, 115.6, 41.2$; HRMS (ESI-TOF) Calcd for $\text{C}_{27}\text{H}_{18}\text{Br}_2\text{ClO}_2^+$ ($[\text{M}+\text{H}]^+$) 566.9357. Found 566.9357.



3l, 1,1'-methylenebis(6-bromonaphthalen-2-ol), offwhite solid: mp 248-249 °C (dec.). ^1H NMR (400 MHz, DMSO) $\delta = 4.68$ (s, 2H), 7.29 (dd, $J = 2.2, 9.2$ Hz, 2H), 7.31 (d, $J = 8.8$ Hz, 2H), 7.62 (d, $J = 8.9$ Hz, 2H), 7.93 (d, $J = 2.1$ Hz, 2H), 8.10 (d, $J = 9.2$ Hz, 2H), 10.41 (s, 2H); ^{13}C NMR (100 MHz, DMSO) $\delta = 152.8, 132.6, 130.3, 130.2, 128.7, 127.4, 126.4, 119.9, 119.7, 115.6, 20.7$; HRMS (ESI-TOF) Calcd for $\text{C}_{21}\text{H}_{15}\text{Br}_2\text{O}_2^+$ ($[\text{M}+\text{H}]^+$) 456.9433. Found 456.9432.

IV. Computational details

Table S1 NPA and MA charges on the carbonyl carbon at different methods

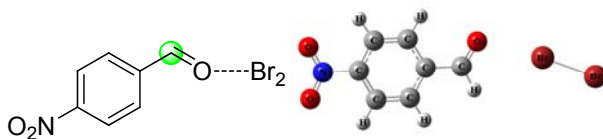


Acid	B3LYP/6-31+G(d,p)		B3LYP/def2-TZVP		M062X/def2-TZVP	
	MA	NPA	MA	NPA	MA	NPA
Br ₂	0.31	0.41	0.12	0.42	0.12 (0.17) ^a	0.43 (0.45) ^a
Br ⁺	0.39	0.43	0.21	0.43	0.25 (0.32) ^a	0.48 (0.51) ^a
I ₂	– ^b	– ^b	0.13	0.42	0.13 (0.16) ^a	0.44 (0.45) ^a
HBr	0.09	0.41	0.11	0.42	0.12 (0.18) ^a	0.43 (0.47) ^a
HI	– ^b	– ^b	0.11	0.42	0.12 (0.15) ^a	0.43 (0.44) ^a
H ₂ SO ₄	0.34	0.42	0.13	0.43	0.16 (0.21) ^a	0.45 (0.48) ^a
TfOH	0.27	0.42	0.13	0.43	0.16 (0.22) ^a	0.46 (0.49) ^a
H ⁺	0.45	0.43	0.19	0.45	0.21 (0.27) ^a	0.49 (0.54) ^a
BF ₃	0.27	0.44	0.15	0.46	0.19 (0.28) ^a	0.48 (0.53) ^a
FeCl ₃	0.22	0.45	0.21	0.46	0.26 (0.33) ^a	0.49 (0.52) ^a
No acid	0.19	0.39	0.09	0.41	0.09 (0.11) ^a	0.42 (0.43) ^a

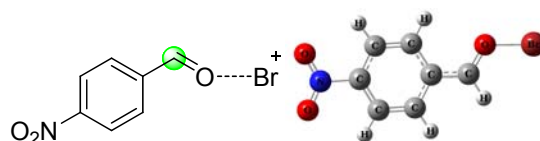
^a Solvent effect was considered, and MeCN served as the solvent.

^b This approach does not apply to I₂ or HI.

Coordinates of all optimized geometries (taking calculations at the M06-2X/def2-TZVP level as example)

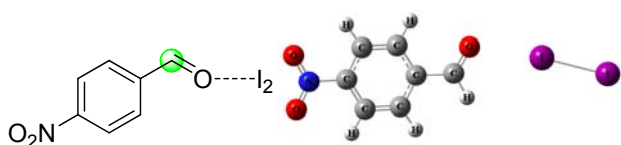


C	-0.43484600	0.40712000	-0.13819700
C	0.93051500	0.58116800	0.02491900
C	1.52656400	1.82234500	0.14214600
C	0.70996900	2.94121400	0.09529600
C	-0.66284800	2.79659100	-0.06778100
C	-1.23606600	1.53198400	-0.18521900
H	-0.84013300	-0.59030000	-0.22380500
H	2.59681600	1.89505600	0.26695700
H	1.14105000	3.93110200	0.18720700
H	-2.30803000	1.45105400	-0.30970600
N	1.79342900	-0.62142100	0.07694600
O	2.98103200	-0.44638300	0.21319200
O	1.25158800	-1.69651600	-0.02034700
C	-1.51956300	4.00530000	-0.10691700
H	-0.99447300	4.97034500	0.01286400
O	-2.71349800	3.97022200	-0.25470800
Br	-3.68976900	6.54332800	0.03002500
Br	-4.27327400	8.75009500	0.30242700

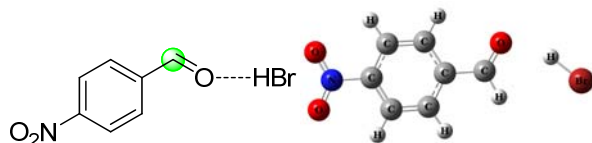


C	-0.53297800	0.53871200	-0.15917300
C	0.84353400	0.65545400	-0.00264100
C	1.51090600	1.85746500	0.15710600
C	0.75813600	3.01393400	0.16192100
C	-0.63894600	2.93209300	0.00595400
C	-1.28564200	1.68902700	-0.15553100
H	-0.97623100	-0.43982900	-0.27841700
H	2.58530600	1.86593000	0.27310900

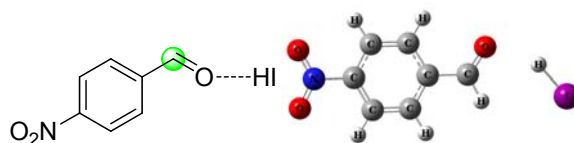
H	1.23849300	3.97698700	0.28579500
H	-2.36021000	1.64441200	-0.27337300
N	1.65423400	-0.59980900	-0.00680200
O	2.84320200	-0.46930600	0.11979700
O	1.04501300	-1.62904200	-0.13642000
C	-1.36065600	4.14554000	0.02360400
H	-0.85168100	5.10106300	0.15525100
O	-2.62547100	4.14139400	-0.11292900
Br	-3.55448600	5.72563200	-0.06967700



C	-4.96032300	-1.09363700	-0.01495400
C	-5.60065700	0.13560000	-0.00709700
C	-4.92605100	1.34122500	0.01998200
C	-3.54061500	1.30890100	0.03965200
C	-2.87197500	0.09012100	0.03218900
C	-3.57875500	-1.11047900	0.00496700
H	-5.54587200	-2.00082600	-0.03634300
H	-5.48122800	2.26729800	0.02466900
H	-2.97644100	2.23372100	0.06022000
H	-3.02922200	-2.04260600	-0.00081500
N	-7.08155800	0.15864800	-0.02958700
O	-7.61940000	1.24046000	-0.02226300
O	-7.65186400	-0.90587700	-0.05373800
C	-1.39122600	0.07709500	0.05056200
H	-0.90094400	1.06737000	0.06706500
O	-0.73509500	-0.93326300	0.04713100
I	2.08617900	-0.39783700	0.01357900
I	4.64538900	0.35370500	-0.02166400

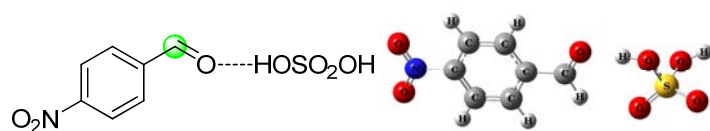


C	-0.50967800	0.48674400	-0.15543200
C	0.85600000	0.66366000	0.00160600
C	1.44624900	1.90360000	0.15586900
C	0.62337000	3.01884600	0.15190900
C	-0.75007900	2.87121600	-0.00467100
C	-1.31767700	1.60766400	-0.15789000
H	-0.91000700	-0.50960600	-0.27135300
H	2.51713100	1.97826100	0.27412200
H	1.04985600	4.00781200	0.27074700
H	-2.39004400	1.52420600	-0.27691600
N	1.72641300	-0.53498200	0.00332700
O	2.91334000	-0.35774900	0.14147800
O	1.19038700	-1.60853700	-0.13381700
C	-1.61129800	4.07502700	-0.00700200
H	-1.09269400	5.04238600	0.12326600
O	-2.80866200	4.03660200	-0.14067200
H	-3.37060300	5.87935300	-0.06256400
Br	-3.23765900	7.30764300	0.06040400

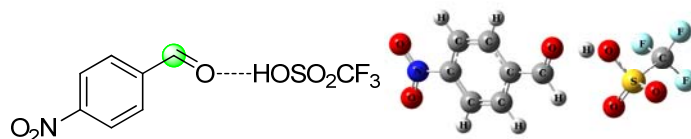


C	-3.31509900	1.19900600	-0.04561200
C	-3.84268900	-0.08235100	-0.00828800
C	-3.06371200	-1.21872200	0.09771000
C	-1.68902900	-1.05862600	0.16663000
C	-1.13224200	0.21467300	0.13219200
C	-1.94281100	1.34291900	0.02673000
H	-3.97845100	2.04719800	-0.12962000
H	-3.53253000	-2.19129500	0.12303500
H	-1.04496300	-1.92637300	0.24640500
H	-1.48012900	2.32087600	0.00067200
N	-5.31274800	-0.24335300	-0.08688600
O	-5.75021500	-1.36871600	-0.04392500
O	-5.97591500	0.76103400	-0.18921300

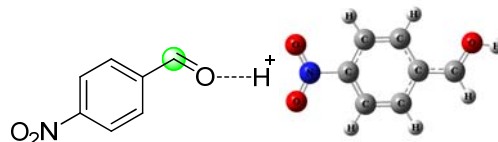
C	0.34088500	0.36372800	0.20294600
H	0.91569800	-0.57944900	0.26149800
O	0.90442000	1.42710100	0.19542300
H	2.94200300	0.91571800	0.13473400
I	4.10961300	-0.18872300	-0.05963500



C	0.01669900	0.73056300	-1.01632600
C	1.00151600	0.90367500	-0.05569400
C	0.97729900	1.91908100	0.88088400
C	-0.08996700	2.80196800	0.85089900
C	-1.09271900	2.65248300	-0.10155100
C	-1.04124000	1.61907500	-1.03573000
H	0.09499700	-0.08430700	-1.72082900
H	1.77428000	2.00362100	1.60447100
H	-0.14689700	3.61087100	1.56928400
H	-1.83547300	1.52653600	-1.76485400
N	2.13658200	-0.04885800	-0.03324000
O	2.98282300	0.11868800	0.81188700
O	2.13788600	-0.92764200	-0.86166200
C	-2.21368800	3.61118400	-0.09479800
H	-2.19609500	4.38912800	0.68126800
O	-3.12431900	3.56794500	-0.89512800
H	-4.37248400	4.61327700	-0.79899700
O	-5.14037500	5.24739100	-0.68117000
S	-4.70069000	6.49336600	0.12297200
O	-4.13007200	7.45410800	-0.99520000
O	-5.86524200	7.08922000	0.66582900
O	-3.57673900	6.15873000	0.92845500
H	-4.86188100	7.94522000	-1.39521300

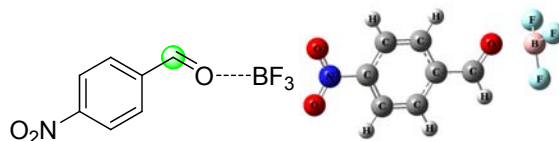


C	-3.85328400	-1.18462900	0.07993600
C	-4.46177600	0.06074700	0.06502900
C	-3.77430000	1.24000500	-0.14941300
C	-2.40700400	1.16345800	-0.35955300
C	-1.76956700	-0.07306900	-0.34879600
C	-2.48930000	-1.24716400	-0.12964400
H	-4.44896200	-2.06869500	0.25372100
H	-4.30544200	2.18012300	-0.14929900
H	-1.83256600	2.06560700	-0.53234100
H	-1.96630000	-2.19440800	-0.12673700
N	-5.92560100	0.13057400	0.29041100
O	-6.43386900	1.22588200	0.28671400
O	-6.50806900	-0.91303800	0.46184100
C	-0.31544900	-0.11794500	-0.57342200
H	0.19570100	0.84010200	-0.74211900
O	0.31734800	-1.15528000	-0.57458900
H	1.85066000	-1.18154000	-0.81984300
O	2.85556300	-1.19870900	-0.98089300
S	3.47263600	0.19260100	-0.75560700
O	4.68608800	0.30259300	-1.47330500
O	2.45648000	1.19417900	-0.82809300
C	3.91484300	0.07110900	1.02339500
F	4.43274600	1.21892800	1.42412400
F	4.78882400	-0.89831900	1.22009900
F	2.81961300	-0.18248800	1.73298500



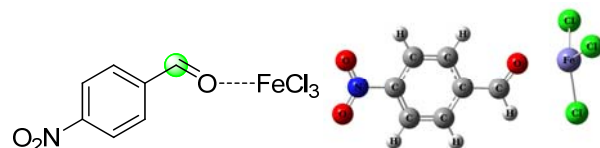
C	-0.54033200	0.54122500	-0.15532000
C	0.83647900	0.66249800	-0.00073300
C	1.50297500	1.86565600	0.16028700

C	0.74756100	3.01912000	0.16684500
C	-0.65097700	2.93517400	0.01156500
C	-1.29591300	1.68940800	-0.14982100
H	-0.98011800	-0.43882200	-0.27526300
H	2.57748700	1.87536100	0.27468100
H	1.22556900	3.98353000	0.29067800
H	-2.37069200	1.64425000	-0.26703000
N	1.65144700	-0.59091900	-0.00958500
O	2.84009100	-0.45588900	0.11372200
O	1.04450900	-1.62114800	-0.13961700
C	-1.37594100	4.13831900	0.02290000
H	-0.86192800	5.09089100	0.14922000
H	-3.05000600	5.03042400	-0.09201300
O	-2.64628900	4.14631300	-0.11357500

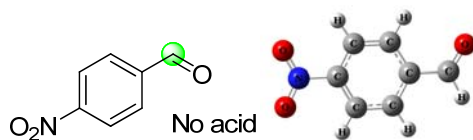


C	-0.89584500	1.25625500	0.00016900
C	0.48210800	1.40149000	-0.04151900
C	1.11931400	2.62730900	-0.06428600
C	0.33144300	3.76618800	-0.04393400
C	-1.05569300	3.65019200	-0.00159300
C	-1.67228800	2.39820900	0.02059700
H	-1.32904600	0.26705100	0.01646800
H	2.19762100	2.67354900	-0.09686100
H	0.79218500	4.74636100	-0.06140000
H	-2.75204400	2.33778300	0.05382300
N	1.31768100	0.17487400	-0.06252200
O	2.51512500	0.32413200	-0.09307200
O	0.73997800	-0.88452700	-0.04745000
C	-1.85635900	4.87186400	0.02031600
H	-1.34050400	5.83836600	0.00264100
O	-3.07664100	4.84783400	0.05811900
B	-4.00228500	6.29449500	0.08167400

F	-4.69824900	6.18767800	-1.06369800
F	-4.69064600	6.15466600	1.22740900
F	-3.04130300	7.25742500	0.09156700



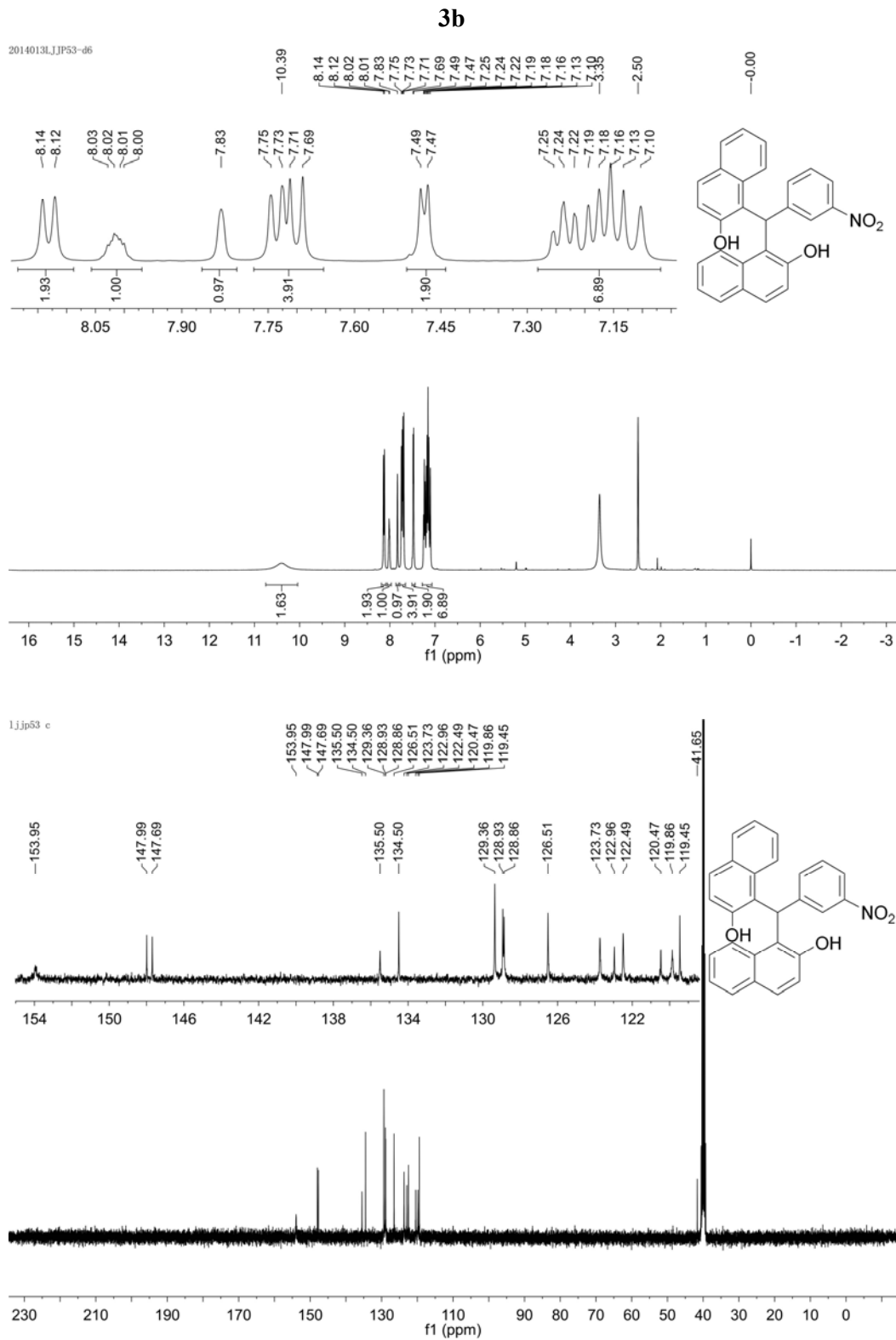
C	3.28627800	-1.14575400	-0.00834700
C	4.12833200	-0.04431800	-0.00321000
C	3.67751500	1.26198000	-0.00613900
C	2.30910800	1.47339800	-0.01464200
C	1.43922700	0.38502800	-0.01893000
C	1.92331400	-0.92460500	-0.01577700
H	3.70688300	-2.14055400	-0.00608300
H	4.38625800	2.07654300	-0.00166000
H	1.91412700	2.48206500	-0.01709100
H	1.22432600	-1.75045300	-0.01917200
N	5.59413700	-0.28103600	0.00614500
O	6.30853500	0.69168000	0.01264400
O	5.96519200	-1.42910000	0.00679100
C	0.00402500	0.64531500	-0.02434100
H	-0.33372100	1.68975400	-0.03110400
O	-0.82542300	-0.25462800	-0.02074400
Fe	-2.87447800	-0.08229700	0.00264700
Cl	-3.46267700	-1.16665600	-1.79074300
Cl	-3.38666800	-0.96257900	1.92666600
Cl	-3.00439800	2.11627800	-0.10521400



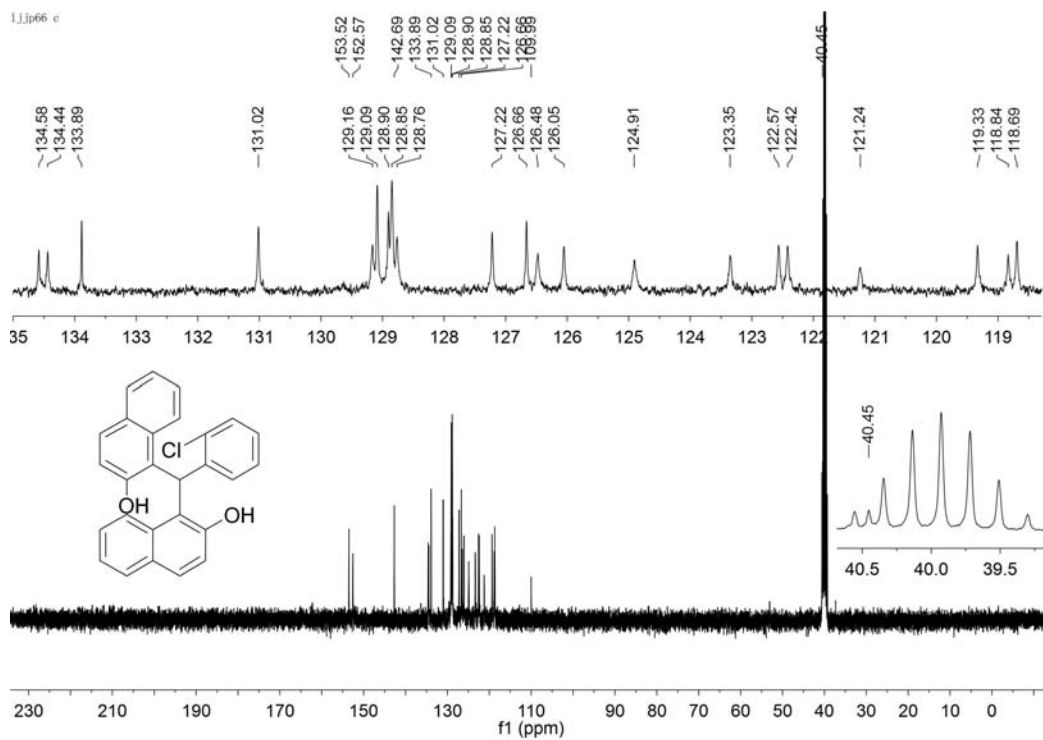
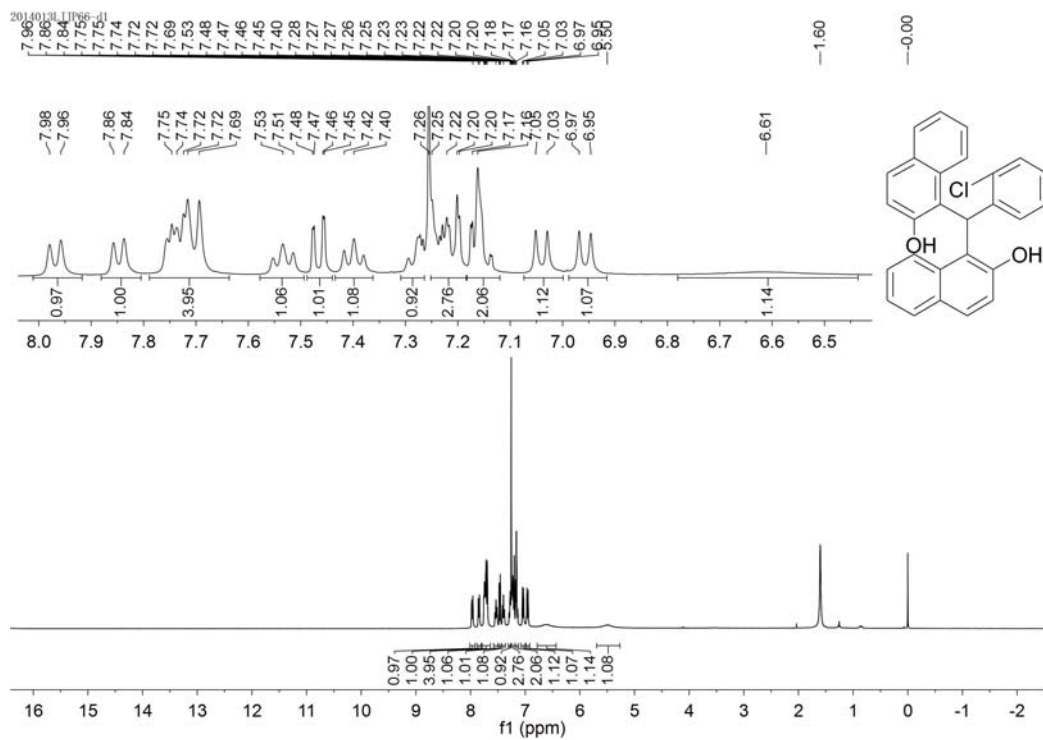
C	-0.52259900	0.53284700	-0.15373600
C	0.85096900	0.63998200	-0.00083500
C	1.50159500	1.84875000	0.15802200
C	0.73397000	3.00295300	0.16298400

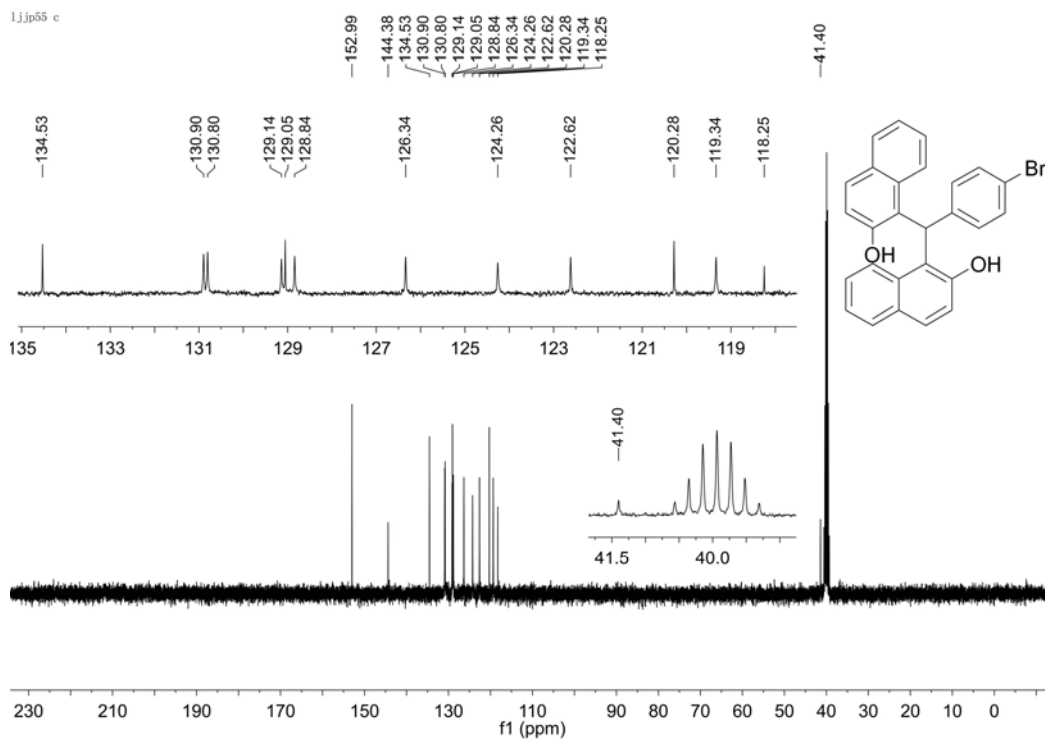
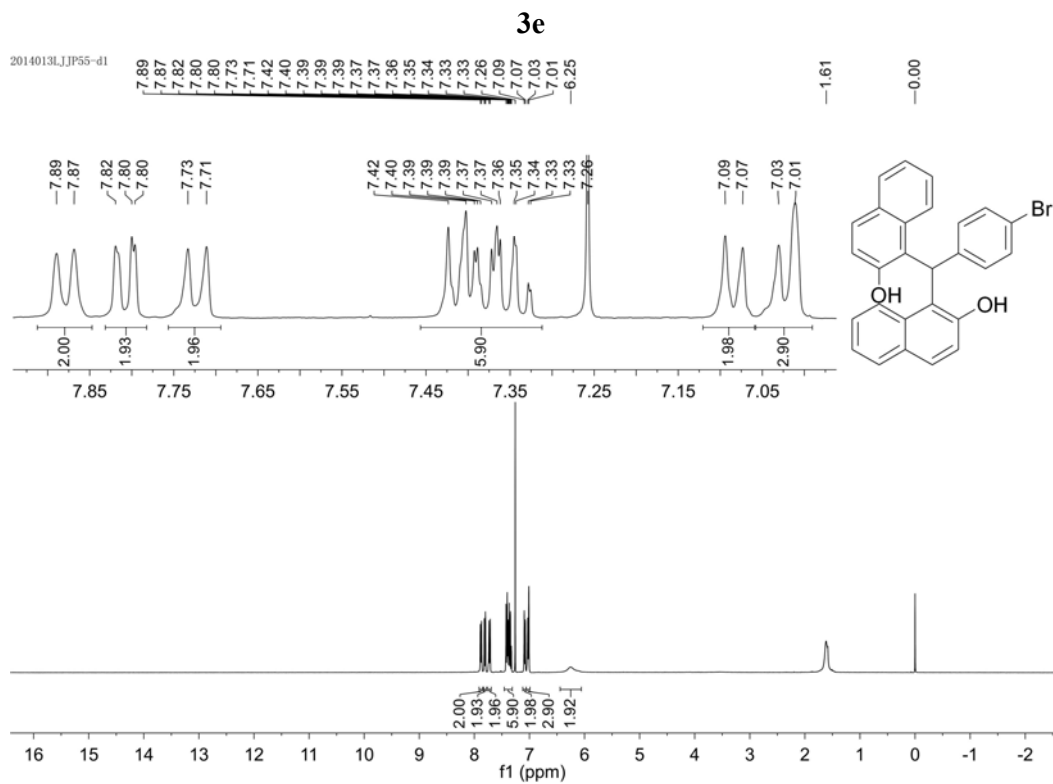
C	-0.64512500	2.92588700	0.01089500
C	-1.27373500	1.69301600	-0.14705600
H	-0.97210100	-0.44187800	-0.27418100
H	2.57507200	1.86984400	0.27294600
H	1.20886000	3.96933000	0.28591600
H	-2.34941400	1.66634200	-0.26287800
N	1.65993200	-0.59965000	-0.00875400
O	2.85593700	-0.48383400	0.12015600
O	1.07099000	-1.64590800	-0.14366300
C	-1.45293300	4.17487600	0.01708100
H	-0.87379900	5.10849000	0.14952200
O	-2.64507500	4.19831600	-0.11038900

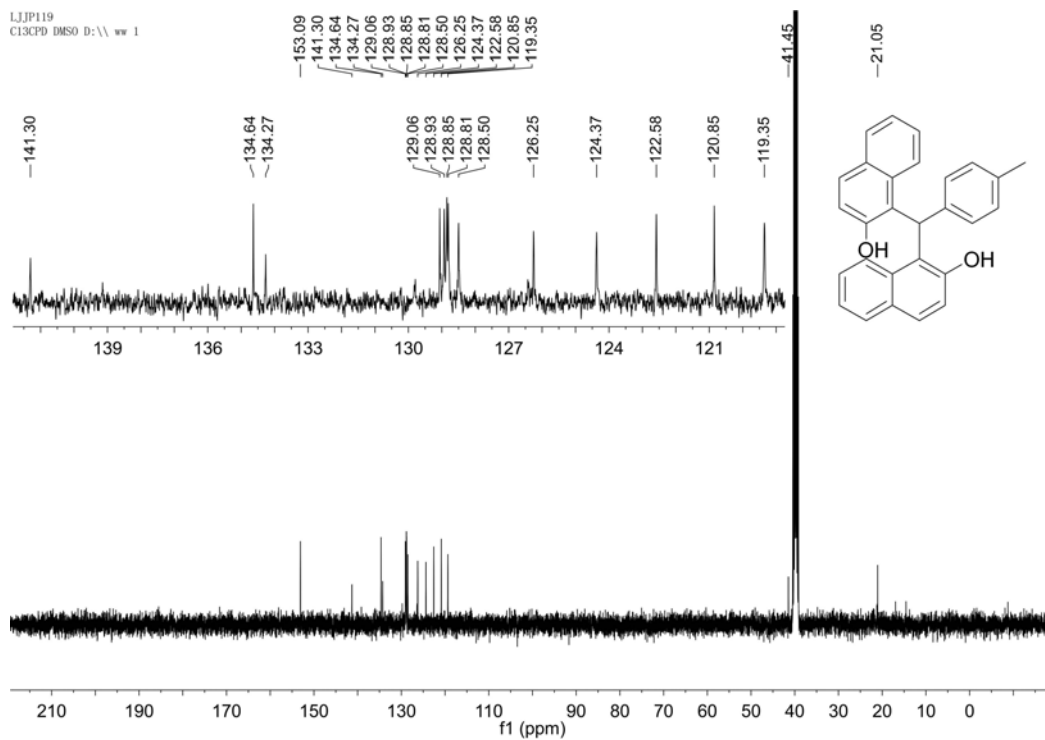
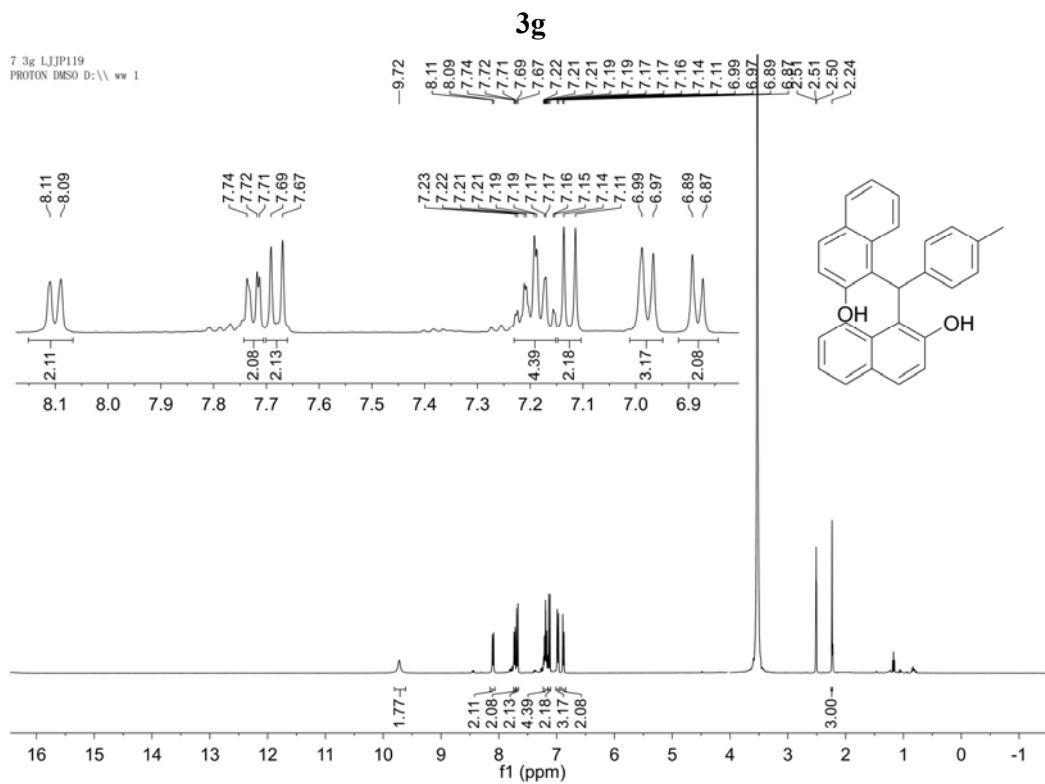
V. Copies of NMR spectra for new compounds

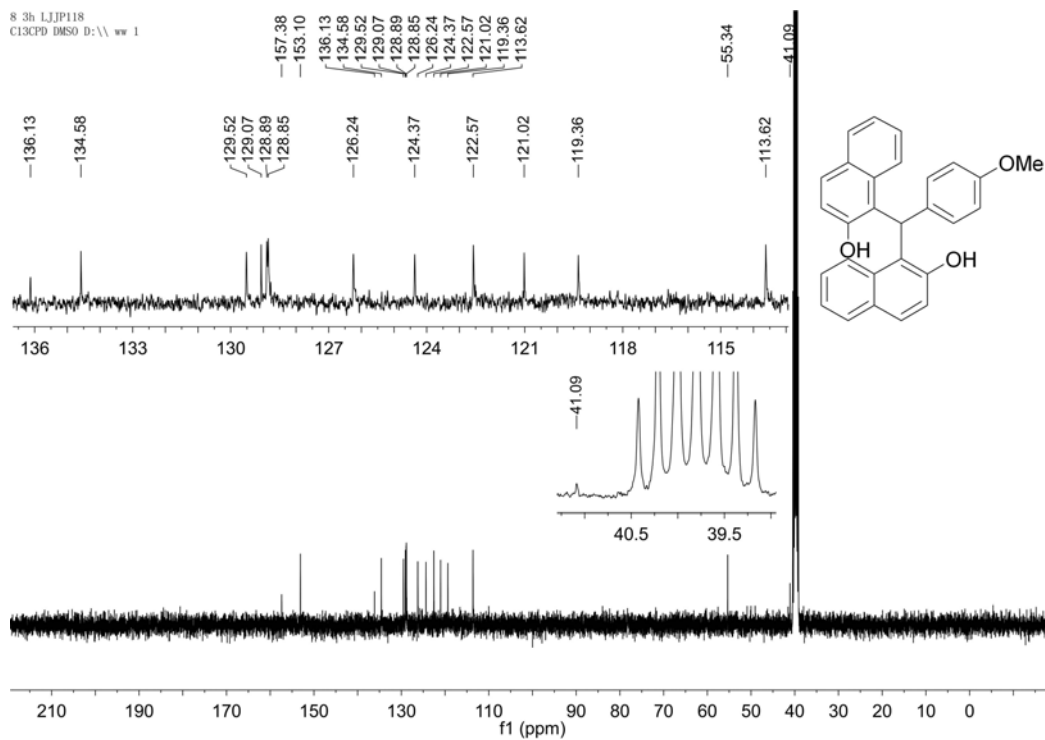
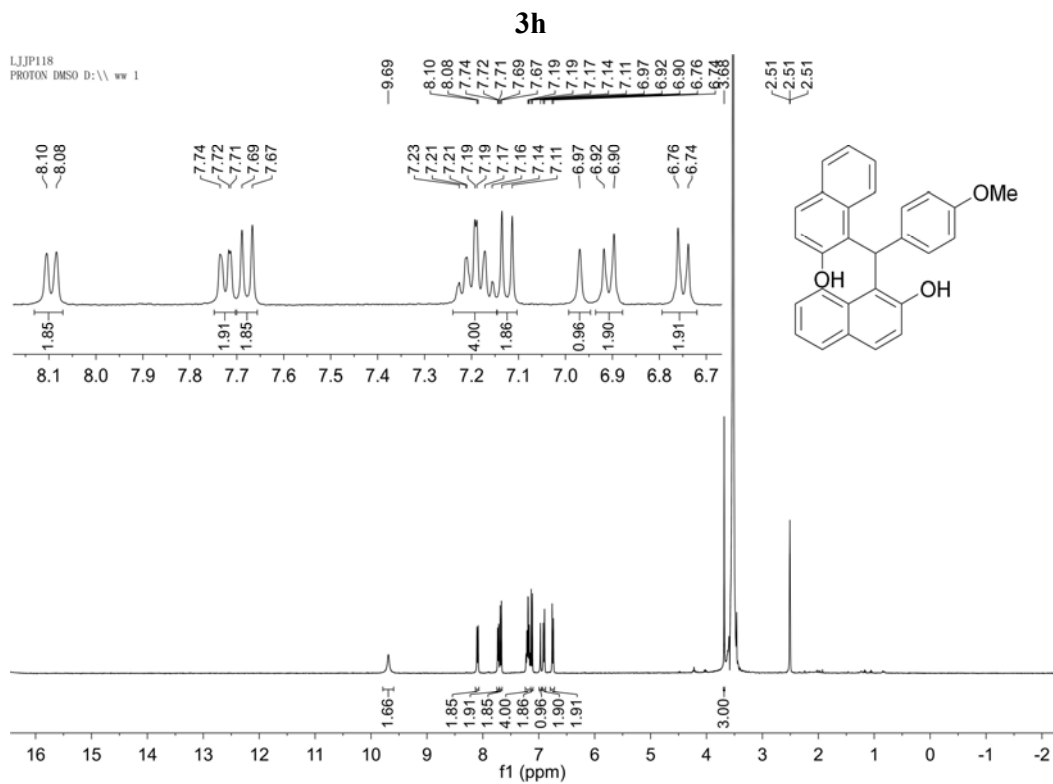


3d



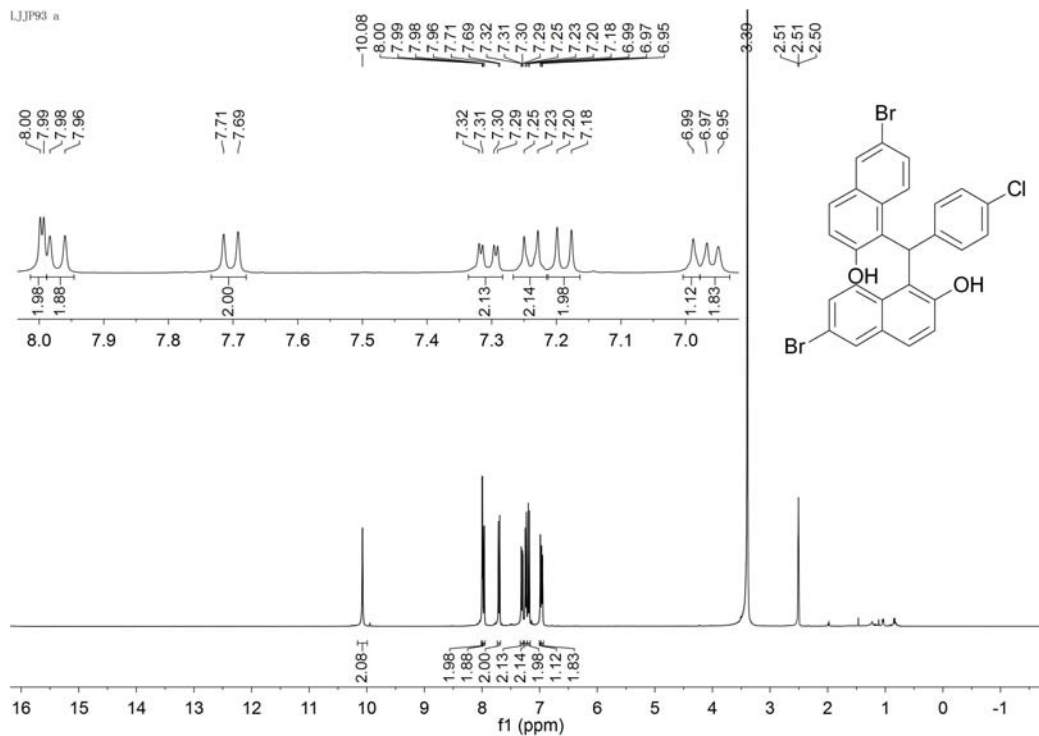




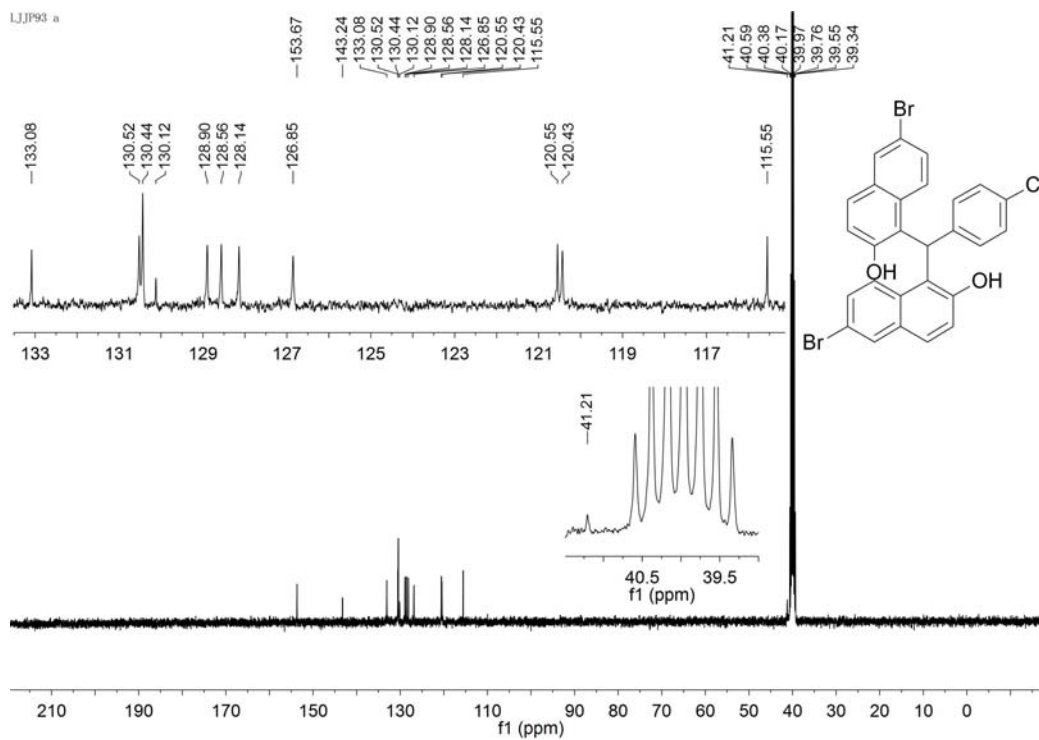


3k

LJJ93 a

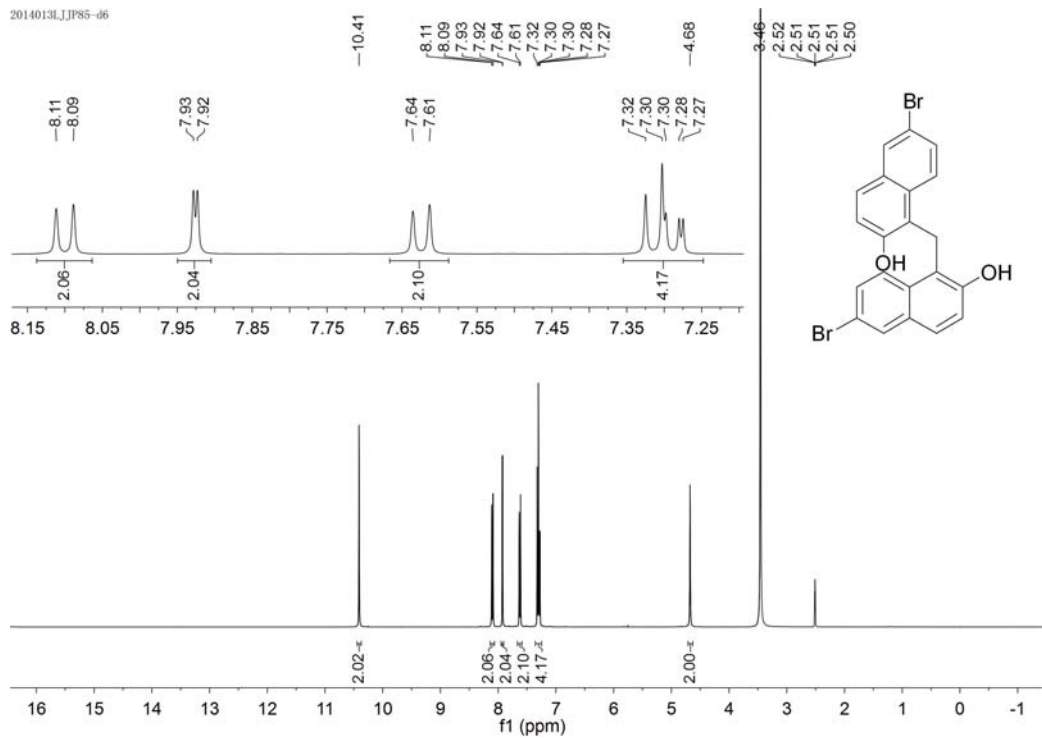


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13 31 C 1jip85-DMSO

